

Methyl pivalate
598-98-1 | DTXSID4027234

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 3.10

Global applicability domain: Inside

Local applicability domain index: 9.84e-01

Confidence level: 8.33e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Benzene</div> <div>Measured: 2.78</div> <div>Predicted: 3.10</div>	<div>Image not found</div> <div>Tetrahydropyran</div> <div>Measured: 3.22</div> <div>Predicted: 3.13</div>	<div>Image not found</div> <div>3-Pentanone</div> <div>Measured: 3.20</div> <div>Predicted: 3.27</div>
<div>Image not found</div> <div>2-Pentanone</div> <div>Measured: 3.19</div> <div>Predicted: 3.27</div>	<div>Image not found</div> <div>Ethyl propionate</div> <div>Measured: 3.15</div> <div>Predicted: 3.27</div>	